Benzene, 1-bromo-2-methoxy-

Other names:	1-bromo-2-methoxybenzene
	2-Bromo-1-methoxybenzene
	2-Bromoanisol
	2-Bromoanisole
	2-Methoxybromobenzene
	2-Methoxyphenyl bromide
	2-bromomethoxybenzene
	NSC 6977
	anisole, o-bromo-
	o-Anisyl bromide
	o-Bromomethoxybenzene
	o-Bromophenyl methyl ether
	o-Methoxybromobenzene
	o-Methoxyphenyl bromide
	o-bromoanisole
Inchi:	InChI=1S/C7H7BrO/c1-9-7-5-3-2-4-6(7)8/h2-5H,1H3
InchiKey:	HTDQSWDEWGSAMN-UHFFFAOYSA-N
Formula:	C7H7BrO
SMILES:	COc1ccccc1Br
Mol. weight [g/mol]:	187.03
CAS:	578-57-4

Physical Properties

Property code	Value	Unit	Source
gf	20.16	kJ/mol	Joback Method
hf	-68.64	kJ/mol	Joback Method
hfus	14.01	kJ/mol	Joback Method
hvap	61.80 ± 1.30	kJ/mol	NIST Webbook
ie	8.30 ± 0.15	eV	NIST Webbook
log10ws	-2.75		Crippen Method
logp	2.458		Crippen Method
mcvol	109.100	ml/mol	McGowan Method
pc	4316.89	kPa	Joback Method
rinpol	1163.00		NIST Webbook
rinpol	1117.00		NIST Webbook
rinpol	1117.00		NIST Webbook
tb	496.20	K	NIST Webbook

tc	711.08	K	Joback Method
tf	289.62	K	Joback Method
vc	0.400	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	194.04	J/mol×K	479.80	Joback Method
cpg	204.18	J/mol×K	518.35	Joback Method
cpg	213.74	J/mol×K	556.89	Joback Method
cpg	222.71	J/mol×K	595.44	Joback Method
cpg	231.12	J/mol×K	633.98	Joback Method
cpg	238.99	J/mol×K	672.53	Joback Method
cpg	246.33	J/mol×K	711.08	Joback Method
dvisc	0.0016504	Pa×s	289.62	Joback Method
dvisc	0.0010390	Pa×s	321.32	Joback Method
dvisc	0.0007108	Pa×s	353.01	Joback Method
dvisc	0.0005176	Pa×s	384.71	Joback Method
dvisc	0.0003956	Pa×s	416.41	Joback Method
dvisc	0.0003141	Pa×s	448.10	Joback Method
dvisc	0.0002571	Pa×s	479.80	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Diffusion coefficients of 2-fluoroanisole, 2-bromoanisole, divinylbenzene and 1,3-divinylbenzene at infinite dilution in supercritical carbon dioxide:	https://www.doi.org/10.1016/j.fluid.2007.07.039
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C578574&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity

gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume